Simulation and Parameter Estimation in Resin-Transfer Mold Filling

Final Report

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1 Overview

This final report summarizes a joint research project between the University of Delaware Center for Composite Materials (CCM), the Advanced Computing and Simulation Division (ACISD) of the Army Research Laboratory (ARL), and the Army High Performance Computing Research Center (AHPCRC). CCM is an established ARO center in materials science research. ACISD is currently supporting an initiative in virtual manufacturing. Under the technical direction of Dr. Kurt Fickie, the research initiative seeks to develop a manufacturing design evaluation capability which will reduce the time required for prototyping new weapon systems utilizing fiber-resin composite materials. Such systems include the Comanche helicopter and the Composite Armored Vehicle (CAV).

The project goal was to complement CCM's leadership role in experimental and analytic composites research with advanced numerical modeling methods and computational resources available through the AHPCRC. The contract provided graduate support and travel for the principal investigator to visit ARL and CCM over a two year period. A total of eight (8) trips were made by the PI to ACISD/APG and CCM. Two research papers were submitted for publication in refereed journals, and a production software system for design evaluation was jointly developed with CCM and ACISD.

2 Statement of Problem

One of the primary design evaluation problems in manufacturing large composite parts is to determine whether the part will be fully saturated by resin under the design injection conditions. The flow of a polymeric fluid through a porous network of fibers is a key phenomenon in the *resin transfer mold filling* (RTM) process.

Numerical simulation of the RTM filling process is necessary for a basic understanding of the process, and for addressing production design needs for large, complex parts. Flow modeling is necessary to predict process variables such as fiber wetting and progression of the free surface flow front. Flow modeling is useful in predicting whether a given model design is feasible (i.e., the part will wet out) and for optimization of the mold design. Some of the properties of mold design which can be optimized during the design process include gate location (a gate is a resin-injection site), number of gates, and flow rates.

Other primary design evaluation problems include the prediction of residual stresses and loading behavior of composite parts. These problems were not addressed by this effort.

3 Summary of Results

The primary research need articulated by ARL and CCM researchers was the fast simulation of isothermal (constant-temperature) mold filling. The problem was that existing simulations were extremely time-consuming because the time complexity tended to grow as $O(n^3)$, where n is the number of nodes in the finite element mesh. Simulation of a part with even a few thousand nodes required many hours. In response to this problem, a new algorithm for solving the isothermal filling problem was developed and embodied in the Fortran code, ISOFIL. The new algorithm involved a novel linear algebra approach to build the Cholesky factorization of the pressure stiffness matrix row by row, rather than reassembling and refactorizing the entire stiffness matrix at each time step. This algorithm reduced the time complexity of the simulation to $O(n^{2.5})$ in theory, with an observed complexity closer to $O(n^2)$. ISOFIL was initially capable of solving 2000-node problems in a matter of a few minutes on IRIS 4D-35 workstations compared to many hours for predecessor codes. More recent improvements to the ISOFIL algorithm and the availability of MIPS R-8000 64-bit processors have reduced the time to a few seconds. ISOFIL remains a production code for numerical simulation of isothermal mold-filling and is undergoing continued enhancement by ARL and University of Minnesota researchers. It can be used on an interactive basis for problems of moderate size ($< 10,000$) nodes.

Simulation of non-isothermal (temperature-varying) flow and the resin curing process requires several rheological parameters – constants appearing in the rate equations describing heat generation and gel conversion. Researchers have observed significant differences in these parameters depending on whether they are obtained in a batch or flow environment. In response to this problem, a graduate student, Robert Duh (Mechanical Engineering, University of Minnesota) developed a parameter estimation methodology for non-isothermal RTM. Duh devised a Lagrangian model of resin flow which captured the important heat and mass-transfer properties of RTM in a one-dimensional flow simulation. He developed an interface between the model and a nonlinear least-squares routine (MINPACK) to estimate rheological

parameters by fitting the model to experimental data on temperature and pressure obtained in RTM molds.

Parameter estimation typically requires many evaluations of the underlying flow model, so there is a need for simplified and fast flow solvers. A concern is that simplified models of flow and thermal transport may miss important heat transfer dynamics. For example, a one-dimensional Lagrangian model neglects diffusion in the axial (flow) direction on the assumption that because the mold is thin, heat transfer through the wall dominates the result (i.e., diffusion through the wall is much greater than in-plane diffusion). A scaling analysis suggested that in-plane diffusion could be important for fast flows. To further test this assumption, a three-dimensional model of heat transfer was developed and solved using the differential-algebraic system solver DASPKF90 on the AHPCRC CM-5. A comparison of three-dimensional results with the one-dimensional model indicated that the assumption of negligible axial heat diffusion was reasonable under standard manufacturing conditions for RTM.

4 Publications and Reports

Two journal publications were prepared under this contract, including,

"A Fast Numerical Method for Isothermal Resin-Transfer Mold Filling," R. Maier, T. Rohaly, S. Advani, K. Fickie, submitted to *Intl. J. Numerical Methods in Engineering*.

"Experimental Estimation of Process Parameters in Resin Transfer Molding," R. Duh, R. Maier, J. Vogel, to appear in *SAMPE Quarterly*.

These manuscripts exist as separate ARO Interim Technical Reports.

5 Personnel and Degrees

Personnel supported by this contract included Robert Duh, Graduate Student, Mechanical Engineering Department, University of Minnesota (Duh's anticipated graduation date is 3/96. His work has been partially supported by this contract), Robert Maier, Staff Scientist, AHPCRC (partial support), and Y.T. Chen, Postdoctoral Fellow, Chemical Engineering and Materials Science Department, University of Minneosta (partial support).

6 Report of Inventions

This work did not result in any patentable inventions. The ISOFIL software is currently distributed and used by ACISD.

References

[1] WALSH, SHAWN M., UNITED STATES OF AMERICA, *IN-SITU SENSOR METHOD AND DEVICE*, patent number 5,210,499, issued May 11, 1993, U.S. Patent Office.

[2] K. MEISSNER AND P. SINCEBAUGH, Preventing mechanical failures in resin transfer molding using embedded sensors and neural networks, preprint, U.S. Army Research Laboratory, Materials Directorate, Watertown MA 02172-0001.

[3] AVNER FRIEDMAN, *Partial Differential Equations of Parabolic Type*, Prentice-Hall, Englewood Cliffs, 1964.

[4] C. L. TUCKER AND R. B. DESSENBERGER, "Governing Equations for Flow through Stationary Fiber Beds," in *Flow and Rheology in Polymer Composites Manufacturing*, ed. S.G. Advani, Elsevier, 1994.

[5] H. P. WANG AND H. S. LEE, "Numerical Techniques for Free and Moving Boundary Problems," in *Fundamentals of Computer Modeling for Polymer Processing*, ed. C.L. Tucker III, Hanser, Munich, 1989.

[6] S. ADVANI AND M. BRUSCHKE A Finite Element/Control Volume Approach to Mold Filling in Anisotropic Porous Media, Polymer Composites, Vol. 11, No. 6, December 1990.

[7] S. ADVANI AND M. BRUSCHKE *Liquid Injection Molding Simulation User's Manual Version 2.0* Center for Composite Materials, University of Delaware, Newark, DE, 19716, December 1992.

[8] S. ADVANI, M. V. BRUSCHKE, AND R. S. PARNAS, "Resin Transfer Molding," in *Flow and Rheology in Polymer Composites Manufacturing*, ed. S.G. Advani, Elsevier, 1994.

[9] W.B. Young, K. Han, L.H. Fong, L. J. Lee, and M.J. Liou, Flow simulation in molds with preplaced fiber mats,*Polymer Composites*, vol. 12, p.391, 1991.

[10] W.B. Young, L. J. Lee, and M.J. Liou. Modification of Control Volume Finite Element Method in Mold Filling Simulation. Report No. ERC/NSM-P-91. NSF Engineering Research Center for Net Shape Manufacturing, The Ohio State University, Columbus, 43210, Jan. 1991.

[11] Alan George a[illegible] Joseph Liu, *Computer Solution of Large Sparse Positive Definite* [illegible]*ems*, Prentice-Hall, Englewood Cliffs, 1981.

[12] SPARSPAK.*NETLIB@ornl.gov*.

[13] Basic Linear Algebra Subroutines.*NETLIB@ornl.gov*.

[14] Thomas J. Hughes. *The Finite Element Method: Linear Static and Dynamic Finite Element Analysis*. Prentice-Hall, Englewood Cliffs, 1987.

[15] J. Crank, *Free a*[illegible] *Moving Boundary Problems*, Oxford University Press, 1984.

[16] B. S. Garbow, K. E. Hillstrom, and J. J. More, "Documentation for MINPACK subroutine LMDIF1."
http://www.netlib.org/minpack/ex/file03 (1980).

[17] V. M. González-Romero, Studies of Reactive Polymer Processing with Fiberglass Reinforcement, PhD thesis, University of Minnesota (1983).

[18] R. S. Hansen. "RTM Processing and Applications." SME Technical Paper EM90-214 (1990).

[19] V. M. González-Romero and C. W. Macosko, Polymer Engineering and Science, 30 (3), 142 (1990).

[20] C. N. Lakakou and S. M. Richardson, Polymer Engineering and Science, 26, 1264 (1986).

[21] J. A. Molnar, L. Trevino, and L. J. Lee, Modern Plastics, 66, 120 (1989).

[22] J. V. Scrivo, Plastics Engineering, 40, 67 (1984).

[23] M. R. Kamal, S. K. Goyal, and E. Chu, AIChE Journal, 34, 94 (1988).

[24] R. Lin, L. Lee, and M. Liou, International Polymer Processing VI, 4, 356 (1991).

[25] S. V. Patankar, Numerical Heat Transfer and Fluid Flow, Hemisphere Publishing Corporation, New York (1980).

[26] J. L. Devore, Probability and Statistics for Engineering and the Sciences, Brooks/ Cole Publishing Company, California (1990).

[27] D. A. Ratkowsky, Handbook of Nonlinear Regression Models, Marcel Dekker, Inc., New York (1990).

[28] D. W. Marquardt, Journal of the Society of Industrial Applied Mathematics, 11, 431 (1963).

[29] R. S. Maier, "A Fast Algorithm for Isothermal Resin-Transfer Mold Filling Simulation," , submitted to *International Journal for Numerical Methods in Engineering* (1993).

[30] P. N. Brown, A. C. Hindmarsh, and L. R. Petzold, SIAM Journal of Scientific Computing, 15, 1467 (1994).